

**Supplemental Table 3.** Variable contribution to the principal components (%) shown in Figure 4. Values higher than 4% are highlighted in yellow.

Variable	PC1	PC2	PC3	Variable	PC1	PC2	PC3
Fucose	0.291	3.484	0.132	Malate	0.850	0.242	6.155
Fructose	0.647	1.967	9.615	Succinate	2.659	0.023	1.194
Fructose-6-P	5.217	0.007	0.096	Alanine	0.237	4.129	0.171
Glucose	1.829	2.295	6.355	$\beta$ -Alanine	2.290	0.713	0.679
Glucoheptose	1.971	0.613	0.016	Asparagine	2.608	0.411	1.571
Isomaltose	5.096	0.106	0.037	Aspartate	0.044	3.529	4.051
1-O-Methyl-mannoside	1.965	0.466	4.423	GABA	0.065	8.775	0.649
Maltose	5.896	0.082	0.000	Glutamate	1.330	5.523	0.017
Raffinose	0.147	0.024	1.175	Glycine	4.063	0.242	0.531
Rhamnose	3.018	0.009	0.575	Isoleucine	4.973	0.066	0.579
Sucrose	1.482	0.365	6.852	Phenylalanine	4.246	0.041	0.982
Trehalose	2.216	0.005	3.815	Proline	3.742	3.007	0.433
Xylose	0.029	1.513	0.707	4-OH-Proline	0.079	6.019	0.551
Galactinol	0.485	0.370	0.051	Serine	3.579	0.062	0.351
Glycerol	2.317	4.423	0.802	Threonine	5.582	0.003	0.287
Myo-inositol	2.727	0.008	4.644	Valine	4.842	0.913	0.448
Maltitol	5.692	0.120	0.046	Hexadecenoic acid	0.170	7.162	0.854
Sorbitol	2.035	0.650	4.496	Octadecanoic acid	0.353	7.519	0.993
Benzoate	1.775	5.986	0.844	Ornithine	0.758	4.766	0.341
Citrate	0.227	0.644	11.429	Phosphate	1.439	0.279	0.171
Dehydroascorbate	2.004	0.181	0.442	Putrescine	0.348	1.421	2.247
2-oxo-Glutarate	0.524	0.146	4.691	cis-3-caffeoylequinic acid	0.007	7.039	0.245
Fumarate	3.542	1.713	1.020	trans-3-caffeoylequinic acid	0.012	6.252	0.592
Glycerate	0.039	0.285	0.632	Spermidine	0.040	0.012	2.152
Gulonate-1,4-lactone	3.620	0.837	0.326	Urea	0.894	2.088	1.127
Quinate	0.005	3.462	9.406				